Light scattering by an elongated particle: spheroid versus infinite cylinder

N V Voshchinnikov† and V G Farafonov‡

† Sobolev Astronomical Institute, St. Petersburg University, Universitetskii pr. 28, St. Petersburg 198504, Russia

‡ St. Petersburg University of Aerocosmic Instrumentation, Bol'shaya Morskaya ul. 67, St. Petersburg 190000, Russia

E-mail: `nvv@astro.spbu.ru`, `far@softjoys.ru`

Abstract. Using the method of separation of variables and a new approach to calculations of the prolate spheroidal wave functions, we study the optical properties of very elongated (cigar-like) spheroidal particles.

A comparison of extinction efficiency factors of prolate spheroids and infinitely long circular cylinders is made. For the normal and oblique incidence of radiation, the efficiency factors for spheroids converge to some limiting values with an increasing aspect ratio a/b provided particles of the same thickness are considered. These values are close to, but do not coincide with the factors for infinite cylinders. The relative difference between factors for infinite cylinders and elongated spheroids ($a/b \gtrsim 5$) usually does not exceed 20 % if the following approximate relation between the angle of incidence α (in degrees) and the particle refractive index $m = n + ki$ takes the place: $\alpha \gtrsim 50|m-1| + 5$ where $1.2 \lesssim n \lesssim 2.0$ and $k \lesssim 0.1$.

We show that the quasistatic approximation can be well used for very elongated optically soft spheroids of large sizes.

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1. Introduction

Rapid calculations of light scattering by non-spherical particles are very important in many scientific and engineering applications (see discussion in [1], [2]). The simplest model of non-spherical particles — an infinitely long circular cylinder is not physically reasonable. However, it looks attractive to find cases when this model could be useful because the calculations for infinite cylinders are very simple. Therefore, we compare the light scattering by *elongated spheroids* and *infinite cylinders*. Previously, such a comparison was made by Martin [3] and Voshchinnikov [4] for normal incidence of radiation (perpendicular to the rotation axis of a particle, $\alpha = 90^{\circ}$).

Our consideration is based on the solution to the light scattering problem for spheroidal particles by the *Separation of Variables Method* (SVM) (see [5], [6] for details). A new type of expansions of the prolate wave functions (Jaffé expansions [7]) opens a possibility to calculate the optical properties of very elongated (cigar-like) particles.

In this paper, we study the optical properties of prolate homogeneous spheroids with large aspect ratios and compare them with those of infinite circular cylinders and of spheroids in quasistatic approximation.

2. Method

2.1. Prolate spheroid

Prolate spheroid is obtained by an ellipse rotation around its major axis. The shape of particle is characterized by the aspect ratio a/b where a and b are the major and minor semiaxes. SVM's solutions to the electromagnetic problem for spheroids published by Asano and Yamamoto [8] and Farafonov [5] (see also [6]) are fundamentally distinguished. In the former, the authors used the Debye potentials to present the electromagnetic fields. This approach is similar to the Mie solution for spheres. Farafonov chose special combinations of the Debye and Hertz potentials, i.e. the potentials used in the solutions for spheres and infinitely long cylinders, respectively. All the electromagnetic fields were divided into two parts: the axisymmetric part not depending on the azimuthal angle φ, and the non-axisymmetric part when the integration over φ gives zero.

The computational efficiency of the Asano and Yamamoto's and Farafonov's solutions can be compared in the following way (see [6] for details). Let N is the number of terms in sums which give the efficiency factors for extinction and scattering $Q_{\rm ext}$, $Q_{\rm sca}$ with some accuracy in the Farafonov's solution. Then, to obtain the results with the same accuracy, the solution of Asano and Yamamoto requires $\approx 2N$ and $\approx 5N$ terms if the aspect ratio $a/b \approx 2$ and $a/b \approx 10$, correspondingly. Because the computational time is proportional to N^3 in this case and $t \propto N^2$ for the Farafonov's solution, the advantage of the latter is evident, especially for large aspect ratios.

It should also be noted that the convergence of Farafonov's solution for spheroids follows that of the Mie solution for spheres (see Table 2 in Voshchinnikov, [9]).

It must be emphasized that the previous calculations for spheroidal particles with the Asano and Yamamoto's solution were restricted by the aspect ratios $a/b \leq 5$ (size parameter $2\pi a/\lambda \leq 30$) [10] or $a/b = 10$ ($2\pi a/\lambda \lesssim 10$) [11].

The particle size can also be specified by the parameters $x_V = 2\pi r_V/\lambda$ (r_V is the radius of a sphere of volume equal to that of spheroid, λ the wavelength of incident radiation) or $c = 2\pi/\lambda \cdot d/2$ (d is the focal distance of a spheroid). The expressions relating different parameters have the form

$$\frac{2\pi a}{\lambda} = c\xi_0 \tag{1}$$

$$x_V = \frac{2\pi r_V}{\lambda} = \frac{2\pi a}{\lambda}\left(\frac{a}{b}\right)^{-2/3} \tag{2}$$

where $r_V^3 = ab^2$. The parameter ξ_0 depends only on the aspect ratio a/b

$$\xi_0 = \left(\frac{a}{b}\right)\left[\left(\frac{a}{b}\right)^2 - 1\right]^{-1/2}. \tag{3}$$

All cross-sections C (extinction, scattering etc) are connected with the corresponding efficiency factors Q via the relation

$$C = GQ \tag{4}$$

where G is the "viewing" geometrical cross-section of a particle (the area of the particle shadow). The factors Q and geometrical cross-sections G depend on the angle of incidence α (the angle between the direction of radiation incidence and the particle rotation axis, $0^0 \leq \alpha \leq 90^0$). The geometrical cross-section of prolate spheroid is

$$G(\alpha) = \pi b\left(a^2\sin^2\alpha + b^2\cos^2\alpha\right)^{1/2}. \tag{5}$$

In the case of oblique radiation incidence ($\alpha \neq 0^0$), the factors depend on the state of polarization of incident radiation: $Q^{\mathrm{TM,\,TE}}$. The superscript TM (TE) is related to the case when the electric vector $\vec{E}$ of the incident radiation is parallel (perpendicular) to the plane defined by the rotation axis of a spheroid and the wave vector. Expressions for the factors can be found in [6].

In order to compare the optical properties of the particles of different shapes it is convenient to consider the ratios of the cross-sections for spheroids to the geometrical cross-sections of the equal volume spheres, $C/\pi r_V^2$. They can be found as

$$\frac{C}{\pi r_V^2} = \frac{[(a/b)^2\sin^2\alpha + \cos^2\alpha]^{1/2}}{(a/b)^{2/3}}\,Q. \tag{6}$$

2.2. Infinite cylinder

The extinction, scattering and absorption cross-sections of an infinite cylinder are, of course, infinite. In order to keep some physical sense the infinite cylinder is replaced by a very-very long finite cylinder and the cross-sections are calculated *per unit length* of an infinite cylinder (see [1], p. 203).

For the infinite circular cylinder, the efficiencies are usually defined as the corresponding cross-sections per unit length, $c_{\rm cyl}$, divided by $2a_{\rm cyl}$, the diameter of the cylinder [12].

For a finite cylinder of length $2L$ and radius $a_{\rm cyl}$, Q is the ratio of the cross-section $C_{\rm cyl}$ to the normally projected geometric area of the cylinder, $2a_{\rm cyl}2L$.

The extinction efficiencies are considered for two cases of polarization of incident radiation: E case (TM mode) and H case (TE mode) [1], [12]

$$Q^E_{\rm ext} = \frac{c^E_{\rm cyl}}{2a_{\rm cyl}} = \frac{C^E_{\rm cyl}}{2a_{\rm cyl}2L} = \frac{2}{x_{\rm cyl}}{\rm Re}\left\{b^E_0 + 2\sum_{n=1}^{\infty} b^E_n\right\} \tag{7}$$

$$Q^H_{\rm ext} = \frac{c^H_{\rm cyl}}{2a_{\rm cyl}} = \frac{C^H_{\rm cyl}}{2a_{\rm cyl}2L} = \frac{2}{x_{\rm cyl}}{\rm Re}\left\{a^H_0 + 2\sum_{n=1}^{\infty} a^H_n\right\} \tag{8}$$

where $x_{\rm cyl} = 2\pi a_{\rm cyl}/\lambda$. The coefficients a^H_n and b^E_n depend on the complex refractive index $m = n + ki$, size parameter $x_{\rm cyl}$ and the angle α ($0^0 < \alpha \leq 90^0$). The expressions for coefficients are given in [12].

Because of different definitions of geometrical cross-sections for spheroids and cylinders, the comparison of factors requires the normalization

$$Q^{\rm TM,\,TE}_{\rm sph} = \frac{Q^{\rm E,\,H}_{\rm cyl}}{\sin\alpha} \tag{9}$$

where $\alpha \neq 0^0$.

3. Numerical results

In previous attempts to find the limits of applications of the model of infinite cylinders ([3], [4]), the particles of the same thickness were considered, i.e. spheroids and cylinders had the equal parameters $2\pi b/\lambda = x_{\rm cyl} = 2\pi a_{\rm cyl}/\lambda$. Martin [3] notes that the extinction factors for spheroids become to resemble those for cylinders if $a/b \gtrsim 4$ for the normal incidence of radiation ($\alpha = 90^0$). But in order to align the peaks in extinction, the x scale for cylinders was stretched by a factor 1.13.

We suggest another way for comparison of the efficiency factors: to put equal the volume and the aspect ratio of a spheroid and a very long cylinder, respectively, i.e.

$$V_{\rm sph} = V_{\rm cyl}, \qquad \frac{a}{b} = \frac{L}{a_{\rm cyl}}. \tag{10}$$

From equation (10), we obtain the relation between the size parameters for infinite cylinder and prolate spheroid

$$\frac{2\pi a_{\rm cyl}}{\lambda} = \frac{2\pi b}{\lambda}\left(\frac{2}{3}\right)^{1/3}. \tag{11}$$

Note that the scaling factor arising in equation (11) $[(3/2)^{1/3} \approx 1.145]$ is close to that found empirically in [3].

3.1. Normal and oblique incidence of radiation

The extinction efficiency factors for spheroids and infinite cylinders are plotted in figure 1 for the case of normal incidence of radiation (perpendicular to the rotation axis, $\alpha = 90°$). There is a *similarity* of the behaviour of the efficiency factors: both TM and TE modes converge to some limiting values which are close to those of infinite cylinders but do not coincide with them. This occurs if the size parameter is defined

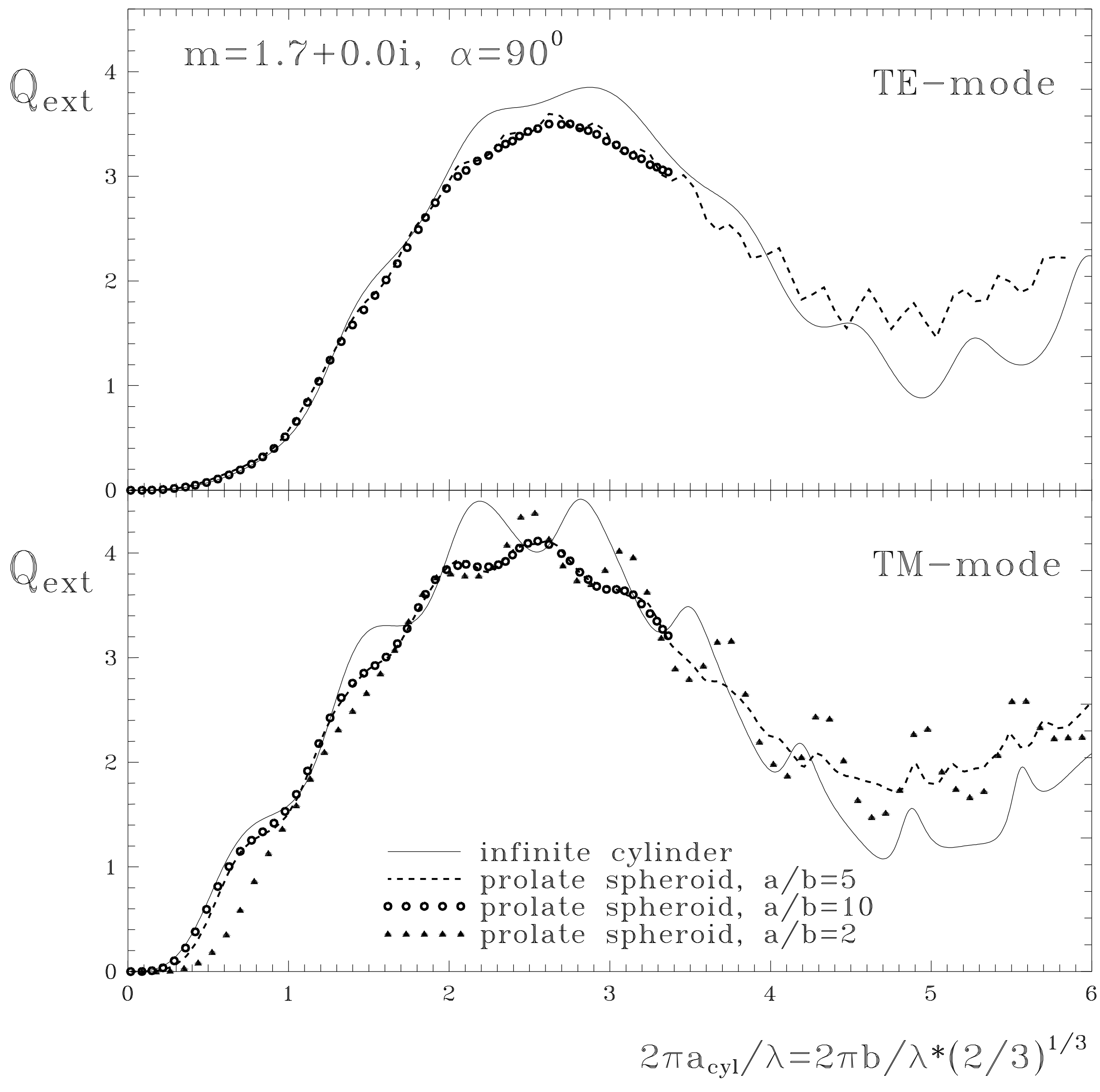

Figure 1. Extinction efficiency factors (TM and TE modes) for prolate spheroids ($Q_{\rm ext} = C_{\rm ext}/G(\alpha)$) and infinite cylinders ($Q_{\rm ext} = C_{\rm ext}/(2a_{\rm cyl} \sin\alpha)$) as a function of the size parameter $2\pi a_{\rm cyl}/\lambda = 2\pi b/\lambda \cdot (2/3)^{1/3}$.

by the relation (11) and the aspect ratio $a/b \gtrsim 5$ (a noticeable difference in factors for $a/b = 2$ it is seen in lower panels of Figs. 1, 2).

If we reduce the angle α (figure 2, upper and middle panels), the similarity in

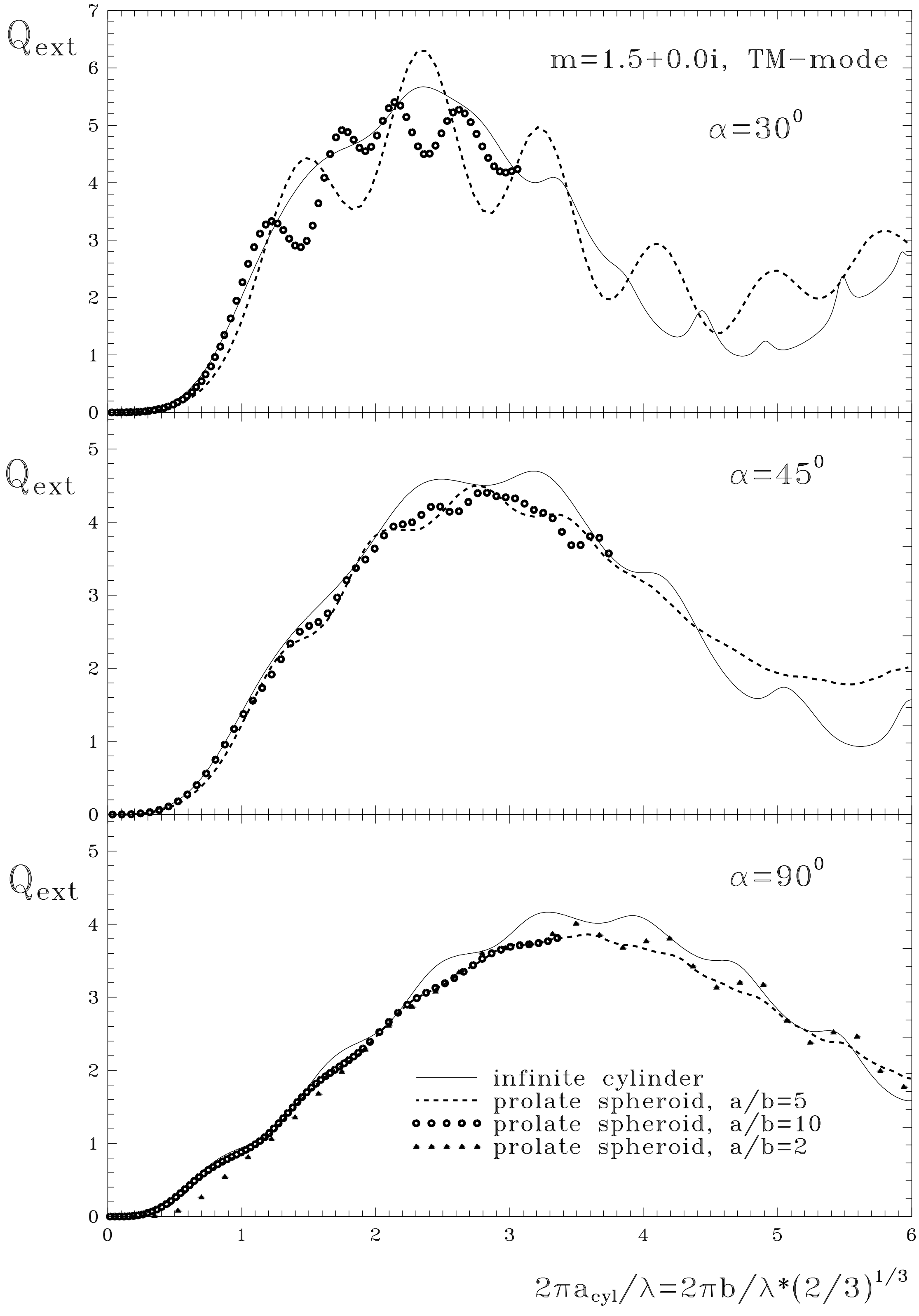

Figure 2. Extinction efficiency factors (TM mode) for prolate spheroids ($Q_{\rm ext} = C_{\rm ext}/G(\alpha)$) and infinite cylinders ($Q_{\rm ext} = C_{\rm ext}/(2a_{\rm cyl}\sin\alpha)$) as a function of the size parameter $2\pi a_{\rm cyl}/\lambda = 2\pi b/\lambda \cdot (2/3)^{1/3}$.

behaviour of factors remains although the ripple-like structure changes. The likeness disappears if we approach the grazing case: the first peak for cylinders occurs at smaller size parameters than for spheroids (see also figure 5). For refractive index $m = 1.5+0.0i$, it takes place if the angle α becomes smaller than $\sim 30^0$. Because the ripples reduce with the decrease of the real part of refractive index n or the increase of its imaginary part k, in these cases the infinite cylinders can be used instead of elongated spheroids at smaller values of α. However, the difference becomes very large for $\alpha \lesssim 15^0$. If $1.2 \lesssim n \lesssim 2.0$ and $k \lesssim 0.1$, the linear relation between the angle of incidence α (in degrees) and the particle refractive index $m = n + ki$ takes the place: $\alpha \gtrsim 50|m-1|+5$. Then the relative discrepancy between factors for infinite cylinders and elongated spheroids ($a/b \gtrsim 5$) does not exceed 20 % near the first maximum.

Anyway, we can expect the resemblance of the extinction properties of very elongated particles (spheroids and cylinders) in the case of radiation incidence close to normal if the size parameters are recalculated according to equation (11).

3.2. Parallel incidence of radiation

Figure 3 shows the extinction efficiency factors for very long spheroids in the case of the incidence of radiation along the rotation axis of the particles. The behaviour of the factors is rather regular, and their values smoothly reduce with the size parameter. There are 25 maxima on the interval $2\pi a/\lambda = 0 - 300$ that is totally distinct from the

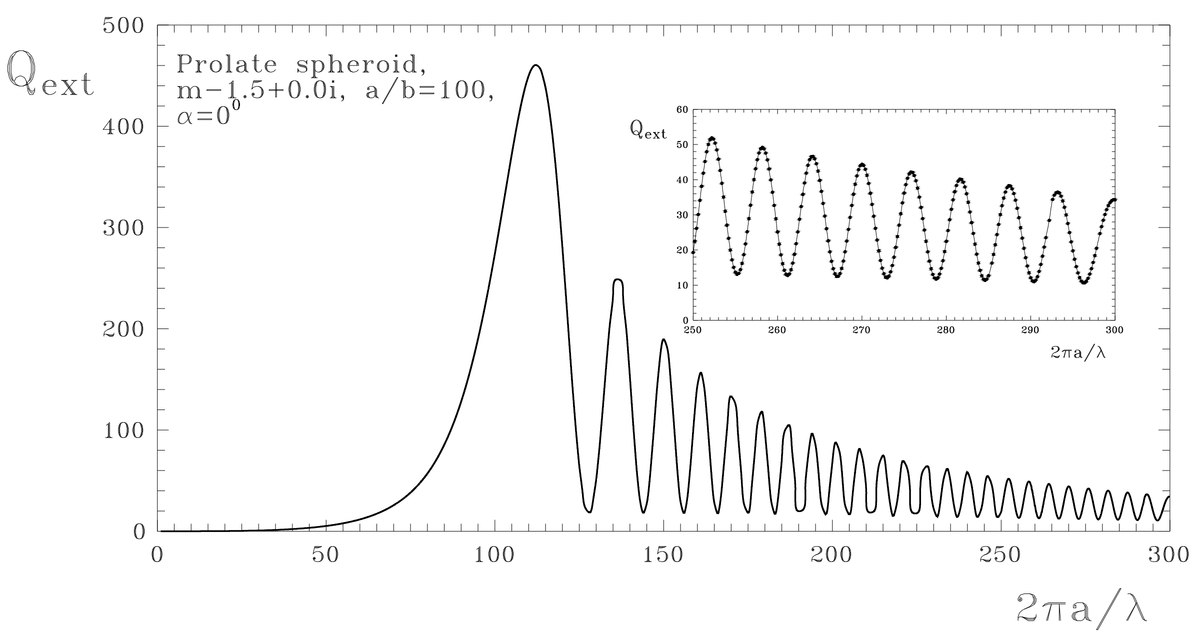

Figure 3. Extinction efficiency factors for elongated spheroidal particles in dependence of size parameter $2\pi a/\lambda$.

extinction by spherical particles (cf. figure 4). The positions of the maxima for large particles are determined by the path of light inside the spheroids (the phase shift of the

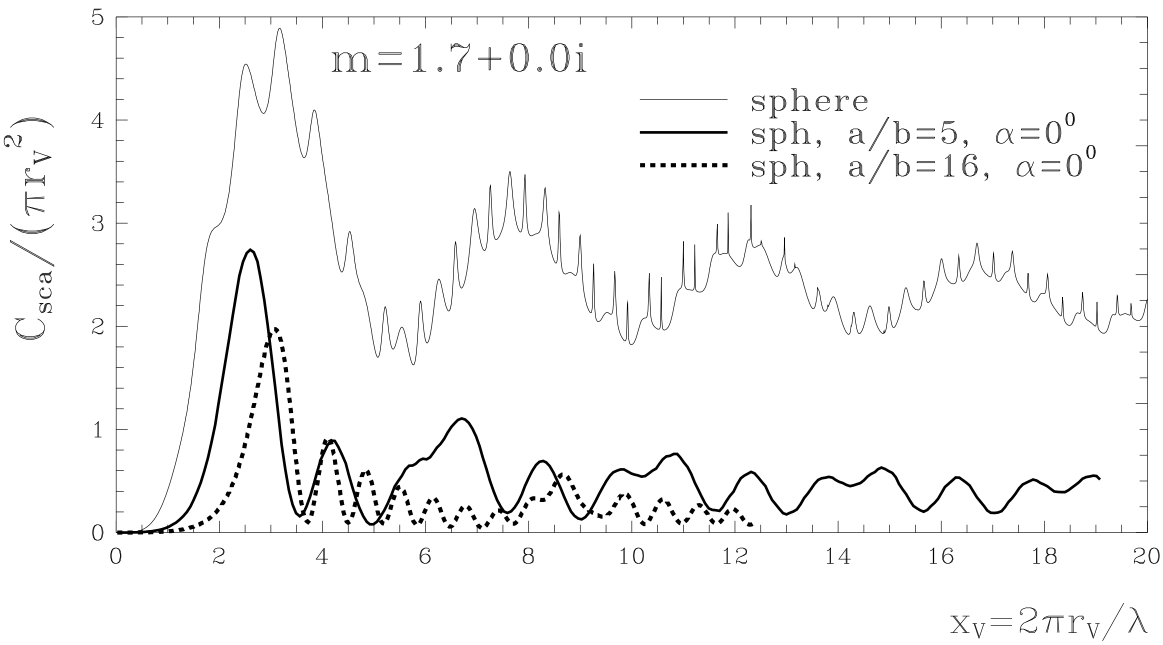

Figure 4. Normalized extinction cross-sections in dependence of the size parameter $2\pi r_V/\lambda$ for spheres and prolate spheroids.

central ray). Note that the "equivolume" size of particles x_V considered on figure 3 is moderate: from equation (2) follows that $x_V \approx 13.92$ if $2\pi a/\lambda = 300$ and $a/b = 100$. But the path of rays inside spheroidal particle is in $300/13.92 \approx 21.5$ times longer in comparison with spherical particle.

The values of factors on figure 3 are very large. This is the result of normalization by geometrical cross-section which is small in this case and is equal to $G(0^0) = \pi b^2$ (see equation (5)). Indicate that the limiting value of extinction factors for particles of any shape must be equal to 2 ("extinction paradox") but as it is seen from the insertion on figure 3, this condition is far to be satisfied although the tendency for reduction of $Q_{\rm ext}$ is observed.

Figure 4 shows the normalized extinction cross-sections for spheres and prolate spheroids at parallel incidence of radiation ($\alpha = 0^0$). As follows from figure 4 spheres of the same volume scatter more radiation than spheroids but the situation changes in the case of another orientation of spheroids. Note also on the absence of ripple-like structure on curves plotted for spheroids.

The ripple-like structure disappear on the extinction curves for cylinders as well in the case of nearly grazing incidence of radiation (figure 5). From figure 5, it is seen that the similarity between elongated spheroids and infinite cylinders is absent. For tangentially incident radiation, the positions and strengths of maxima for infinite cylinders do not coincide with those for spheroids at $\alpha = 0^0$.

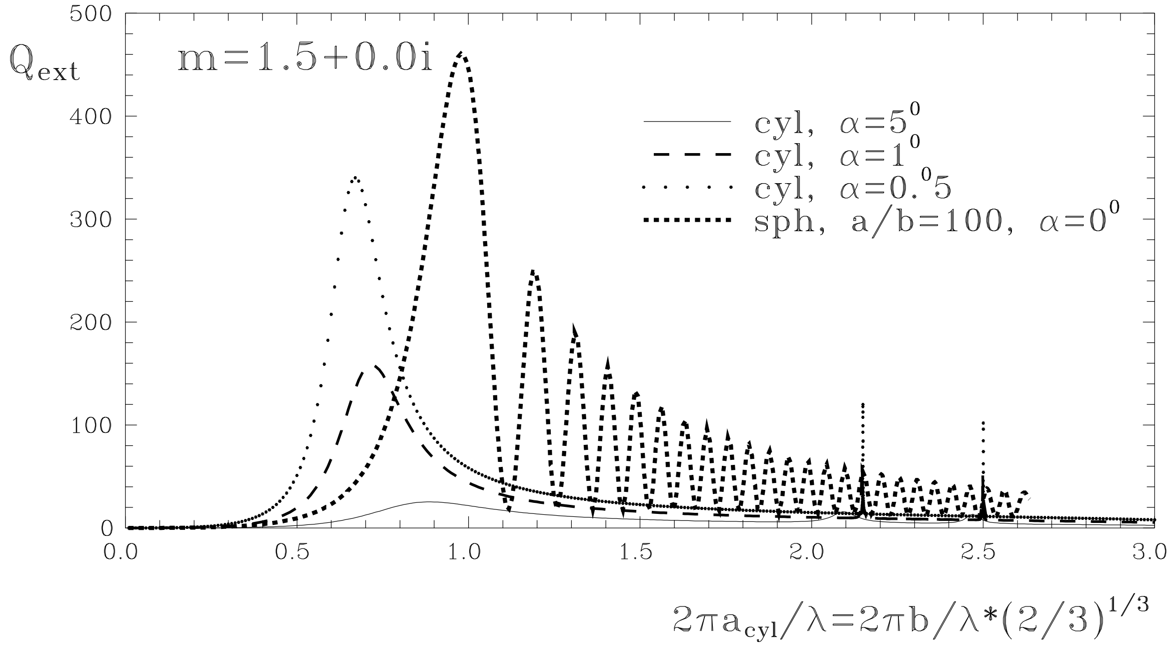

Figure 5. Extinction efficiency factors (TM mode) for prolate spheroids ($Q_{\rm ext} = C_{\rm ext}/G(\alpha)$) and infinite cylinders ($Q_{\rm ext} = C_{\rm ext}/(2a_{\rm cyl}\sin\alpha)$) as a function of the size parameter $2\pi a_{\rm cyl}/\lambda = 2\pi b/\lambda \cdot (2/3)^{1/3}$.

3.3. Quasistatic approximation

The optical properties of extremely prolate and oblate particles may be approximately calculated using the *quasistatic approximation*. This is a generalization of the Rayleigh and Rayleigh-Gans approximations when the electromagnetic field inside a particle is replaced by the incident radiation field (as in the Rayleigh-Gans approximation), taking into account the polarizability of the particle (as in the Rayleigh approximation). The expressions for the efficiency factors and amplitude matrices were obtained in [13]. The range of validity of the quasistatic approximation is discussed in [14].

Figures 6 and 7 show the extinction efficiency factors for spheroids calculated with the exact solution and the quasistatic approximation in the case of normal ($\alpha = 90^0$) and parallel ($\alpha = 0^0$) incident radiation. As we consider non-absorbing particles, the extinction efficiencies coincide with the scattering ones which are in the quasistatic approximation:

$$Q_{\rm sca}^{\rm TM}(0^0) = \frac{c^4\xi_0^2(\xi_0^2-1)}{9\pi}|\tilde{\alpha}_1|^2 \int_0^{2\pi}\int_0^{\pi} (\sin^2\varphi + \cos^2\theta\cos^2\varphi)\, G^2(u)\sin\theta {\rm d}\theta {\rm d}\varphi \tag{12}$$

$$Q_{\rm sca}^{\rm TM}(90^0) = \frac{c^4\xi_0^2(\xi_0^2-1)}{9\pi}|\tilde{\alpha}_3|^2 \int_0^{2\pi}\int_0^{\pi} G^2(u)\sin^3\theta {\rm d}\theta {\rm d}\varphi \tag{13}$$

where $\tilde{\alpha}_1$ and $\tilde{\alpha}_3$ are the polarizabilities,

$$G(u) = \frac{3}{u^3}(\sin u - u\cos u) \tag{14}$$

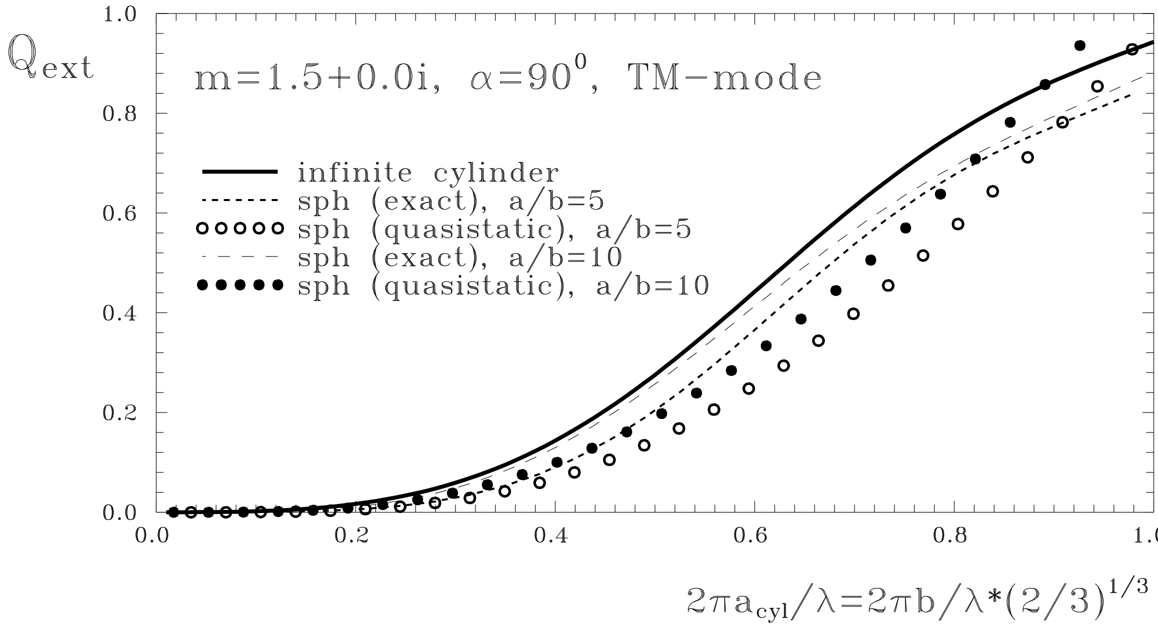

Figure 6. The extinction efficiencies for prolate spheroids and infinite cylinders. The results for spheroids were calculated using exact solution and quasistatic approximation.

and

$$u = c\xi_0 \sqrt{(\cos\theta - 1)^2 + \left(\frac{a}{b}\right)^{-2} \sin^2\theta} \tag{15}$$

if $\alpha = 0^0$ and

$$u = c\xi_0 \sqrt{\cos^2\theta + \left(\frac{a}{b}\right)^{-2} (\sin^2\theta + 1 - 2\sin\theta\cos\varphi)} \tag{16}$$

if $\alpha = 90^0$.

Figure 6 shows the enlarged part of figure 2 (lower panel) for small size parameters. Here, the results for quasistatic approximation are also plotted. It is seen that this approximation describes rather well the behaviour of efficiencies for relatively large size parameters (the value $2\pi a_{\rm cyl}/\lambda = 1$ corresponds to $2\pi a/\lambda = 5.725$ for $a/b = 5$ and $2\pi a/\lambda = 11.45$ for $a/b = 10$).

The extinction efficiencies for optically soft particles are drawn in figure 7. The results given here show the light scattering by a spheroidal cavity ($m_{\rm cavity} = 1.49 + 0.0i$) in glass ($m_{\rm medium} = 1.48 + 0.0i$). As follows from figure 7, the quasistatic approximation allows to calculate the optical properties with the relative error smaller than $\sim 25\,\%$ in a wide range of particle sizes.

The range of validity of the quasistatic approximation is discussed in [14]. It was found that a maximum parameter x_V for which the quasistatic approximation and exact theory yielded the results coinciding within 1%, can be described by the following

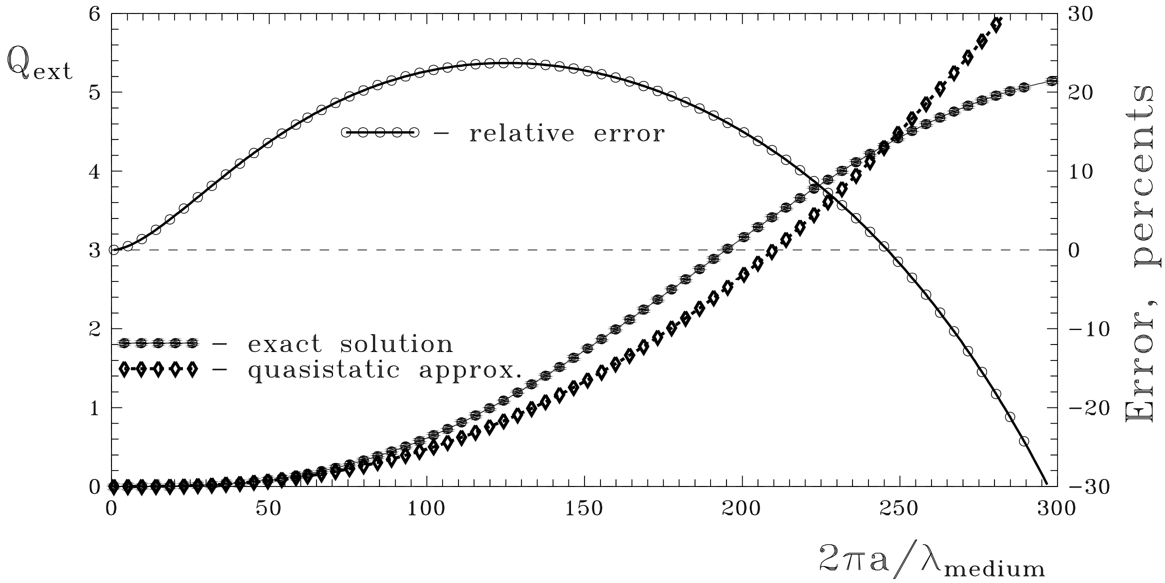

Figure 7. The extinction efficiency factors (left y-axis) for prolate spheroids ($m_{\mathrm{medium}} = 1.48 + 0.0i$, $m_{\mathrm{cavity}} = 1.49 + 0.0i$, $a/b = 10$, $\alpha = 0^0$) in dependence of the size parameter $2\pi a/\lambda_{\mathrm{medium}}$. The calculations were made using exact solution and quasistatic approximation. The relative error of the calculations of factors in quasistatic approximation is given by the right y-axis.

approximate formulae:

$$x_V \lesssim \frac{0.02\ln(a/b) + 0.13}{(n-1)^{0.30}} \tag{17}$$

for prolate spheroids and $\alpha = 0°$,

$$x_V \lesssim \frac{0.10}{(n-1)^{0.13\ln(a/b)+0.29}} \tag{18}$$

for prolate spheroids and $\alpha = 90°$,

$$x_V \lesssim \frac{0.11}{(n-1)^{0.09\ln(a/b)+0.26}} \tag{19}$$

for oblate spheroids and $\alpha = 0°$,

$$x_V \lesssim \frac{0.06\ln(a/b) + 0.12}{(n-1)^{0.23}} \tag{20}$$

for oblate spheroids and $\alpha = 90°$.

4. Conclusions

We applied a new method of calculations of the spheroidal wave functions to the study of the optical properties of very elongated (cigar-like) spheroids. New approach allowed to compare light scattering by prolate spheroids and infinitely long circular cylinders

and investigate the applicability of the quasistatic approximation for very elongated spheroids.

It is found that the efficiency factors for spheroids and cylinders have quite similar behaviour for the normal and oblique incidence of radiation, if the aspect ratio of spheroids $a/b \gtrsim 5$. The resemblance of factors arises provided spheroids and very long cylinders of the same volume and aspect ratio are considered. The following approximate relation between the angle of incidence α (in degrees) and the particle refractive index $m = n + ki$ takes the place: $\alpha \gtrsim 50|m-1| + 5$ where $1.2 \lesssim n \lesssim 2.0$ and $k \lesssim 0.1$. In this case, the relative discrepancy between factors for infinite cylinders and elongated spheroids ($a/b \gtrsim 5$) does not exceed 20 % near the first maximum.

It is shown that the quasistatic approximation rather well describes the extinction by very elongated optically soft spheroids of large sizes.

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